

# DENSITY DEPENDENCE, TRIPLET CORRELATION AND DIFFERENT POTENTIALS EFFECT ON THE SINGLE EXCITATION SPECTRUM IN LIQUID $^4\text{He}$

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Using Brillouin-Wigner (BW) perturbation formula, we analysed density and different potentials effect in the maxon and roton part of the single excitation spectrum in liquid  $^4\text{He}$ . In addition having two different forms of the three body structure factor we derived the influence of the triplet correlations. The most impressive result is that the term, with three phonon states, in the second order of BW formula significantly depends upon density. This is what has been anticipated by our earlier research. We also found that the differences among the used potentials appeared at higher densities.

## 1. Introduction

After the precise neutron inelastic scattering experiments of Cowley and Woods<sup>1)</sup> it has been shown that Landau phonon-roton spectrum is only a part of the excitation spectrum in liquid helium 4. A schematic depiction of the observed spectrum in  $^4\text{He}$  is shown in Fig. 1 from Ref. 2. There are two branches. The upper branch has two roton nature and it is called multiparticle branch. This branch corresponds to exciting two (or more) quasiparticles from the condensate. For wave vectors greater than  $2 \cdot 10^{10} \text{ m}^{-1}$  its mean energy approaches the free particle energy  $\hbar^2 k^2 / 2m$ . The lower branch for wave vectors less than  $2.6 \cdot 10^{10} \text{ m}^{-1}$ , may be thought of as corresponding to the excitations of a single quasiparticle from the condensate.

The single-excitation spectrum has been studied for a long time<sup>3-8)</sup>. Brillouin-Wigner (BW) perturbation theory has been used very successfully<sup>4-8)</sup>.

Firstly for the energy of elementary excitations we used the relation

$$\varepsilon(k) = \varepsilon_0(k) + \varepsilon_{2a}/(1 - \varepsilon_3/\varepsilon_{2a}). \quad (1)$$

This relation was obtained and studied in Refs. 7 and 8. The notations are as follows:

$$\varepsilon_0 = \frac{\hbar^2 k^2}{2m S_k}, \quad (2)$$

$$\varepsilon_{2a} = \frac{1}{2} \sum_l' \frac{|\langle k | W | k-l, l \rangle|^2}{a_l}, \quad (3)$$

$$\varepsilon_3 = \frac{1}{4} \sum_l' \sum_{l'}' \frac{\langle k | W | k-l, l \rangle \langle k-l, l | W | k-l', l' \rangle}{a_l} \times \frac{\langle k-l', l' | W | k \rangle}{a_{l'}}, \quad (4)$$

$$W = H - E_0 - \varepsilon_0(k), \quad (5)$$

$H = -\frac{\hbar^2}{2m} \sum_i \Delta_i + V$  is the hamiltonian of the system,  $E_0$  is the ground state energy,  $\varepsilon(k) = E - E_0$  is excitation energy,

$$a_l = \varepsilon(k) - \varepsilon_0(l) - \varepsilon_0(|\vec{k} - \vec{l}|). \quad (6)$$

For the basis of the perturbation procedure we took Jackson-Feenberg (JF) one- and two-phonon functions

$$|k\rangle = \frac{1}{\sqrt{N S_k}} \varrho_k |\psi_0\rangle, \quad (7)$$

$$|k-l, l\rangle = \frac{1}{\sqrt{N^2 S_k S_{k-l}}} \varrho_k \varrho_{k-l} |\psi_0\rangle, \quad \text{all } l \neq 0, k. \quad (8)$$

$\varrho_k$  is the Fourier component of the density operator.  $S_k$  is the two body structure factor

$$S_k = \frac{1}{N} \langle \psi_0 | \varrho_k \varrho_{-k} | \psi_0 \rangle. \quad (9)$$

The expressions  $\varepsilon_{2a}$  and  $\varepsilon_3$  suitable for integration read<sup>8)</sup>

$$\varepsilon_{2a} = \frac{1}{8\pi \varrho_0} \int_0^\infty dl \cdot l^2 \int_{-1}^1 dt \frac{1}{S_k S_l S_{k-l}} \frac{F(k, l, t)^2}{a_l}, \quad (10)$$

$$\varepsilon_3 = \frac{1}{4(2\pi)^3 \rho^2 S_k} \int_0^\infty dl l^2 \int_0^\infty dl' l'^2 \int_{-1}^1 dt \int_{-1}^1 dt' \int_0^{2\pi} d\varphi \int_0^{2\pi} d\varphi' \times$$

$$\times \frac{1}{S_{k-l} S_{k-l'} S_l S_{l'}} \frac{F(k, l, t)}{a_l} \frac{F(k, l', t')}{a_{l'}} G(k, l, l'), \quad (11)$$

where

$$F(k, l, t) = \frac{\hbar^2}{2m} \{ (k^2 - k l t) S_l + k l t S_{k-l} - \frac{k^2}{S_k} S_3(k, -k-l, l) \}, \quad (12)$$

$$G(k, l, t) = -\frac{\hbar^2}{2m} \{ (l l' T S_3(k-l, -k+l', l-l') + (k l t - l l' T) \times$$

$$\times S_3(k-l, -l', -k+l+l') + (k l' t' - l l' T) S_3(-k+l', l, k-l'-l) \}, \quad (13)$$

$$T = t \cdot t' + \sqrt{(1-t^2)(1-t'^2)} \cdot \cos(\varphi - \varphi'), \quad (14)$$

$S_3$  and  $S_4$  are three- and four-body structure factors.

Secondly, as we found that at higher densities the formula (1) gives slightly better results than the pure BW formula up to the second order, we enlarged our basis (7–8) for the three-phonon function

$$|k-m, m-n, n\rangle = \frac{1}{\sqrt{N^3 S_{k-m} S_{m-n} S_n}} \varrho_{k-m} \varrho_{m-n} \varrho_n |\psi_0\rangle \quad \text{all } \vec{m}, \vec{n} \neq 0, \vec{k} \quad (15)$$

and used the pure BW formula

$$\varepsilon_0 = \varepsilon_0(k) + \varepsilon_{2a} + \varepsilon_{2b}, \quad (16)$$

where

$$\varepsilon_{2b} = \frac{1}{6} \sum'_m \sum'_n \frac{|\langle k|W|k-m, m-n, n\rangle|^2}{a_{mn}} \quad (17)$$

and

$$a_{mn} = \varepsilon(k) - \varepsilon_0(k-m) - \varepsilon_0(m-n) - \varepsilon_0(n).$$

Thirdly, in order to obtain the influence of the terms of higher order in BW perturbation formula we also included some of the third and fourth order terms; namely we solved the equation

$$\varepsilon = \varepsilon_0 + \varepsilon_{2a} + \varepsilon_{2b} + \varepsilon_{3a} + \varepsilon_{4a}, \quad (18)$$

where

$$\varepsilon_{3a} = \frac{1}{2} \sum'_m \sum'_n \frac{\langle k|W|k-m, m\rangle}{a_m} \times \frac{\langle m|W|m-n, n\rangle \langle k-m, m-n, n|W|k\rangle}{a_{mn}}, \quad (19)$$

$$\varepsilon_{4a} = \frac{1}{2} \sum'_m \sum'_n \frac{|\langle k|W|k-m, m\rangle|^2 |\langle m|W|m-n, n\rangle|^2}{a_m^2 a_{mn}}. \quad (20)$$

The matrix elements contained in the relations (17, 19, 20) were obtained in Ref. 5.

In this paper we considered density dependence, triplet correlation and different potentials effects on the single particle excitation spectrum in the maxon and roton part of wave vectors. In Sec. 2 we defined our approximations and performed the corresponding calculations. Sec. 3 includes discussion of our results.

## 2. A choice of the approximation and numerical computation

Eq. (1) for energy  $\varepsilon$  is an integral equation. It includes two and six dimensional integrals. The integrands in this expression contain two-, three- and four-body structure factors. We do not know their exact form. Two body structure factor has been calculated by Campbell and coworkers as a function of particle density at zero temperature<sup>9)</sup>. This quantity has also been studied in many experiments at temperatures different from zero<sup>1,10)</sup>. Three body structure factor has been analysed by JF, who introduced the convolution approximation (CA) of this quantity<sup>4)</sup>

$$S_3^c(-k, l, k-l) = S_{-k} F_l S_{k-l}. \quad (21)$$

Later on the function  $S_3$  has been considered by others<sup>7,11-14)</sup>. A very simple but generalized form of  $S_3$  has been defined in Refs. 13 and 14 (we call it Feenberg form)

$$\begin{aligned} S_3^F(-k, l, k-l) &= (k^2/S_k + l^2/S_l + |\vec{k} - \vec{l}|^2/S_{k-l})^{-1} \times \\ &\times \left\{ \frac{1}{2}(k^2 + l^2 + |\vec{k} - \vec{l}|^2) S_3^c + \frac{1}{2}(|\vec{k} - \vec{l}|^2 - k^2 - l^2) \times \right. \\ &\left. \times (S_l + S_k - S_{k-l}) + l^2 S_k + k^2 S_l \right\}. \quad (22) \end{aligned}$$

It is worth to notice, as shown in Ref. 13, that the relation (22) is transformed into (21) if pure triplet correlations are neglected in the ground state wave function

$$\psi_0(1, 2, \dots, N) = \exp \left\{ \sum_{i < j} u_2(r_i, r_j) + \sum_{i < j < k} u_3(r_i, r_j, r_k) \right\}. \quad (23)$$

Triplet correlations are described by  $u_3$  term and Jastrow's by  $u_2$ .

Four body structure factor is known in the convolution approximation<sup>7,12)</sup>

$$S_4^c = S_l S_{l'} S_{k-l'} S_{k-l} \{ S_k + S_{l-l'} + S_{k-l-l'} - 2 \}. \quad (24)$$

We notice that functions  $S_3$  and  $S_4$ , in the above mentioned approximations, depend upon the two body structure factor.

In order to obtain the solution of Eq. (1) we employed the CA and Feenberg approximation of function  $S_3$ . The reason for this choice is that these two approximations have been already studied and because of their well known relation with the ground state wave function in  $x$ -representation. The four-body structure factor was also used in the convolution approximation.

Numerical analysis of integral equation (1) was performed by the successive iteration method. Two dimensional integrals, appearing in relation (10), were computed by 32 point Gauss quadrature, and six dimensional integrals, included in  $\epsilon_3$ , were calculated by the number theoretic method<sup>15)</sup>. The number of particles  $\rho$  is included explicitly in  $\epsilon$  and also implicitly through the structure factors.

In our calculation we concentrated on the maxon and roton part of the spectrum. We used two body structure factors which have been obtained by Chang and Campbell<sup>9)</sup> for Lennard-Jones potential. This quantity has been theoretically obtained at densities 2.185, 2.388, 2.571 and 2.844 ( $10^{27} \text{ m}^{-3}$ ) in two forms:  $S_J(k)$  and  $S(k)$ .  $S_J(k)$  has been obtained from the optimum Jastrow trial function within the hypernetted chain approximation;  $S(k)$  includes the effect of triplet correlation in the ground state wave function.

The relation (1) was firstly solved taking  $\epsilon_3 = 0$ . It was done, among other things, in order to compare our calculation with that from Ref. 6. Our results are shown in Table 1. The results of the calculation of complete relation (1) are given in Table 2. In order to save computing time, we calculated excitation energy, in this case, only for the values of the wave vector  $k$  which correspond to the maximum and minimum values in Table 1 (except for the roton at density  $2.185 \cdot 10^{28} \text{ m}^{-3}$ ).

TABLE 1.

$k(10^{10} \text{ m}^{-1})$	$\rho(10^{28} \text{ m}^{-3})$							
	2.185		2.388		2.571		2.844	
0.9						(24.819)		
1.0	19.599	(23.233)	20.697	(24.686)	21.626	(25.801)*	22.879	(27.396)*
1.1	19.902	(23.353)	20.869	(24.564)	21.703	(25.546)	22.902	(26.852)
1.2	20.395	(23.692)*	21.298*	(24.754)*	22.095*	(25.677)	23.305*	(26.815)
1.3	20.306	(22.815)	21.066	(23.560)	21.757	(24.175)	22.373	(24.929)
1.4	20.542*	(22.392)	21.225	(22.947)	21.864		22.781	(23.923)
1.5	20.218	(20.895)	20.715	(21.089)	21.192		21.866	(21.287)
1.7	19.947	(18.552)						
1.8	19.926**	(17.635)	19.748	(16.909)	19.544	(16.176)	19.212	(14.928)
1.9	20.076	(17.058)**	19.692**	(16.116)**	19.290**	(15.174)**	18.599**	(13.625)**
2.0	20.746	(17.190)	20.320	(16.238)	19.897	(15.299)	19.215	(13.760)
2.1	22.336	(18.286)	21.715	(17.359)	21.284	(16.442)	20.625	(14.918)
2.2	24.265	(20.325)	23.914	(19.498)	23.559	(18.642)	23.007	(17.206)
2.3	26.984	(23.184)	26.849	(22.623)	26.722	(22.039)	26.531	(20.953)

Maxon and roton part of single excitation spectrum in convolution (Feenberg) approximation of the three body structure factor calculated from pure BW relation  $\epsilon = \epsilon_0(k) + \epsilon_{2a}(k)$  and  $S = S_J(S_k)$  for Lennard-Jones potential. Energy is given in  $10^{-23} \text{ J}$ . The signs \* and \*\* denote the maximum and minimum among output numbers in maxon-roton part of the spectrum respectively.

TABLE 2.

$k(10^{10}\text{m}^{-1})$	$\rho(10^{28}\text{m}^{-3})$							
	2.185		2.388		2.571		2.844	
1.0	(22.202)				(25.328)		(27.356)	
1.1			20.742 (23.914)		21.604		22.951	
1.2								
1.3								
1.4	20.062							
1.9	20.167	(17.542)	19.743	(16.394)	19.318	(15.313)	18.614	(13.473)

The energy corresponding to the maximum of maxon- and minimum of roton-part of the spectrum from Table 1, calculated from expression (1) for  $S = S_J(S_R)$  in CA (Feenberg) approximation. Units are the same as in Table 1.

Eq. (16) was solved using the same numerical procedure as in Eq. (1). The matrix element in  $\varepsilon_{2b}$  includes three-phonon function and was approximated by the Lee and Lee form<sup>5)</sup>. Again all integrands depend on the two-body structure factor. We used the structure factor for six potentials obtained in Ref. 9: Lennard-Jones (LJ), Bruch-McGee (BM), Farrar-Lee (FL), Beck (B), Aziz et al. (A) and Maitland-Smith (MS). For three-body structure factor  $S_3$  we took the Feenberg form. After the numerical integration we constructed a parabolic interpolation and obtained extreme point on these curve  $k_{ex}$  and  $\varepsilon_{ex}$ . The results are presented in Table 3.

Eq. (18) was again solved in the same way but only for the Aziz potential and several densities. For input wave vectors we used the »maximum« and »minimum« values from Table 3. The results are given in Table 4.

### 3. Discussion

Let us analyse the results from Tables 1 and 2. Considering the density dependence of the roton gap  $\Delta_0$ , we see from Table 1 that in CA it slightly decreases with the increase of density. This result does not confirm the conclusion from Ref. 6. The same qualitative behaviour is found for the Feenberg approximation of  $S_3$ , but with values closer to the experimental ones<sup>16)</sup>. Thus we found that the inclusion of the triplet correlation in the ground state wave function and the application of the Feenberg approximation of  $S_3$  improve the density dependence of the roton spectrum.

Qualitative behaviour in the maxon part of the spectrum, when density increases, in both approximations is the same. The Feenberg approximation of  $S_3$  again shows better agreement with the experimental results<sup>16)</sup>.

A comparison of the density dependence of the double energy of the roton minimum ( $2\Delta_0$ ) with the density dependence of the single excitation energy at the maximum ( $\Delta_1$ ) of the maxon part of spectrum shows that only in the Feenberg approximation we find the same qualitative behaviour as the one measured in the experiment<sup>16)</sup>. Namely, one maxon could break up into two rotons for the density

TABLE 3.

$q$	$k$	$\epsilon_0$	$\epsilon_{2a}$	$\epsilon_{2b}$	$\epsilon$	$k_{cx}$	$\epsilon_{cx}$	
LJ	2.185	1.1	31.362	-7.819	-1.127	22.416	1.173	22.762
		1.2	32.193	-8.585	-1.192	22.717		
		1.3	31.865	-8.813	-1.314	21.738		
	2.388	1.99	26.466	-8.061	-3.815	14.590	1.998	14.583
		2.0	25.701	-8.076	-3.042	14.583		
		2.1	27.390	-8.611	-3.184	15.595		
	2.571	1.1	33.432	-8.652	-1.208	23.572	1.160	23.834
		1.2	34.345	-9.341	-1.289	23.715		
		1.3	33.211	-9.385	-1.440	22.386		
	2.844	1.9	24.101	-7.558	-3.315	13.228	1.962	13.0015
		2.0	24.408	-7.693	-3.627	13.088		
		2.1	26.184	-8.282	-3.768	14.134		
	2.185	1.1	35.295	-9.496	-1.304	24.495	1.154	24.745
		1.2	36.093	-10.131	-1.401	24.561		
		1.3	34.467	-9.985	-1.583	22.899		
2.844	1.9	22.929	-7.268	-3.922	11.739	1.964	11.472	
	2.0	23.254	-7.422	-4.279	11.553			
	2.1	25.133	-8.079	-4.406	12.648			
1.946	0.9	36.071	-9.284	-1.295	25.492	1.006	26.325	
	1.0	38.207	-10.525	-1.360	26.322			
	1.1	38.226	-11.034	-1.520	25.672			
2.185	1.9	21.224	-7.003	-5.161	9.060	1.966	8.757	
	2.0	21.632	-7.203	-5.592	8.837			
	2.1	23.665	-7.975	-5.676	10.017			
BM	1.946	1.1	28.985	-7.453	-1.112	20.420	1.166	20.681
		1.2	29.914	-8.119	-1.180	20.615		
		1.3	29.202	-8.269	-1.306	19.627		
	2.185	1.8	23.962	-7.481	-2.446	14.035	1.890	13.652
		1.9	23.873	-7.485	-2.731	13.657		
		2.0	24.972	-7.822	-2.925	14.225		
	2.388	1.1	33.710	-9.725	-1.560	22.425	1.156	22.641
		1.2	34.641	-10.460	-1.666	22.515		
		1.3	33.646	-10.529	-1.857	21.260		
	2.388	1.9	23.967	-8.228	-4.361	11.378	1.984	10.858
		2.0	23.953	-8.258	-4.819	10.876		
		2.1	25.709	-8.871	-4.999	11.839		
	2.388	1.1	38.225	-12.197	-2.050	23.978	1.154	24.211
		1.2	39.268	-13.032	-2.192	24.044		
		1.3	37.982	-13.003	-2.455	22.524		
2.388	2.0	23.566	-8.829	-7.155	7.5815	2.054	7.317	
	2.1	24.305	-9.153	-7.641	7.511			
	2.2	27.103	-10.222	-7.614	9.267			

DŽELALIJA AND KILIĆ: DENSITY DEPENDENCE . . .

$\rho$	$k$	$\varepsilon_0$	$\varepsilon_{2a}$	$\varepsilon_{2b}$	$\varepsilon$	$k_{cx}$	$\varepsilon_{cx}$		
FL	2.571	1.1	42.561	-14.825	-2.576	25.160	1.151	25.378	
		1.2	43.679	-15.754	-2.751	25.174			
		1.3	42.234	-15.659	-3.079	23.496			
	2.0	2.0	23.732	-9.549	-9.804	4.379	2.110	2.987	
		2.1	23.352	-9.474	-10.879	2.999			
		2.2	25.293	-10.305	-11.078	3.910			
	1.946	1.0	1.0	27.812	-6.465	-0.969	20.378	1.127	20.766
			1.1	29.025	-7.251	-1.026	20.748		
			1.2	29.547	-7.805	-1.101	20.641		
		1.8	1.8	23.859	-7.370	-2.244	14.518	1.880	14.227
			1.9	24.158	-7.417	-2.496	14.245		
			2.0	25.331	-7.776	-2.671	14.884		
	2.180	1.0	1.0	32.323	-8.406	-1.330	22.587	1.104	22.828
			1.1	33.543	-9.296	-1.419	22.828		
			1.2	34.055	-9.907	-1.528	22.620		
1.9	1.9	24.275	-8.107	-3.899	12.269	1.976	11.877		
	2.0	24.391	-8.182	-4.293	11.916				
	2.1	26.165	-8.789	-4.457	12.919				
2.388	1.0	1.0	36.719	-10.667	-1.749	24.303	1.086	24.513	
		1.1	38.082	-11.707	-1.867	24.508			
		1.2	38.516	-12.352	-2.019	24.145			
1.9	1.9	24.998	-9.023	-5.612	10.363	2.049	8.704		
	2.0	24.023	-8.740	-6.397	8.886				
	2.1	24.794	-9.065	-6.837	8.892				
2.571	1.0	1.0	41.037	-13.064	-2.181	25.792	1.062	25.879	
		1.1	42.385	-14.205	-2.332	25.848			
		1.2	42.902	-14.930	-2.516	25.456			
2.0	2.0	24.179	-9.424	-8.732	6.023	2.106	4.833		
	2.1	23.896	-9.388	-9.671	4.837				
	2.2	25.826	-10.187	-9.886	5.753				
1.946	1.0	1.0	27.358	-6.140	-0.930	20.315	1.138	20.705	
		1.1	28.534	-6.903	-0.956	20.675			
		1.2	29.149	-7.499	-1.023	20.627			
	1.8	1.8	24.391	-7.303	-2.036	15.052	1.873	14.816	
		1.9	24.472	-7.365	-2.260	14.847			
		2.0	25.660	-7.722	-2.417	15.521			
2.180	1.0	1.0	31.712	-7.995	-1.230	22.487	1.110	22.805	
		1.1	32.995	-8.887	-1.306	22.802			
		1.2	33.487	-9.488	-1.406	22.593			
1.9	1.9	24.611	-8.003	-3.530	13.078	1.969	12.785		
	2.0	24.823	-8.100	-3.881	12.842				
	2.1	26.542	-8.673	-4.048	13.821				

DŽELALIJA AND KILIĆ: DENSITY DEPENDENCE...

$\rho$	$k$	$\varepsilon_0$	$\varepsilon_{2a}$	$\varepsilon_{2b}$	$\varepsilon$	$k_{ex}$	$\varepsilon_{ex}$	
<b>B</b>								
2.388	1.0	35.930	-10.042	-1.614	24.274	1.095	24.577	
	1.1	37.378	-11.085	-1.717	24.576			
	1.2	37.792	-11.722	-1.855	24.215			
	2.045	1.9	25.312	-8.903	-5.020	11.389	2.045	9.973
		2.0	24.479	-8.675	-5.696	10.108		
		2.1	25.270	-8.997	-6.092	10.181		
	2.571	1.0	40.057	-12.117	-1.921	26.019	1.082	26.211
		1.1	41.515	-13.268	-2.045	26.202		
		1.2	42.06	-13.979	-2.208	25.819		
2.101		2.0	24.605	-9.260	-7.425	7.920	2.101	6.951
		2.1	24.341	-9.253	-8.197	6.951		
		2.2	26.294	-10.004	-8.407	7.883		
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1.946	1.0	27.539	-6.341	-0.949	20.249	1.134	20.675	
	1.1	28.778	-7.126	-1.004	20.648			
	1.2	29.332	-7.687	-1.076	20.569			
	1.879	1.8	24.327	-7.380	-2.164	14.783	1.879	14.505
		1.9	24.353	-7.425	-2.405	14.523		
		2.0	25.485	-7.765	-2.577	15.143		
2.180	1.0	31.953	-8.239	-1.307	22.407	1.108	22.770	
	1.1	33.322	-9.167	-1.387	22.768			
	1.2	33.768	-9.763	-1.495	22.510			
	1.976	1.9	24.472	-8.115	-3.769	12.588	1.976	12.214
		2.0	24.587	-8.183	-4.152	12.252		
		2.1	26.297	-8.759	-4.326	13.212		
<b>A</b>								
2.388	1.0	36.397	-10.429	-1.699	24.269	1.088	24.410	
	1.1	37.658	-11.433	-1.817	24.408			
	1.2	38.271	-12.131	-1.955	25.185			
	2.049	1.9	25.206	-9.010	-5.371	10.825	2.049	9.203
		2.0	24.230	-8.727	-6.122	9.381		
		2.1	25.316	-9.373	-6.554	9.389		
	2.571	1.0	40.443	-12.718	-2.130	25.595	1.076	25.727
		1.1	41.859	-13.871	-2.273	25.715		
		1.2	42.450	-14.619	-2.448	25.383		
2.106		2.0	24.354	-9.406	-8.383	6.565	2.106	5.453
		2.1	24.114	-9.382	-9.275	5.457		
		2.2	25.974	-10.143	-9.513	6.318		
<hr/>								
1.962	1.1	29.026	-7.215	-1.026	20.785	1.151	2.0825	
	1.2	29.694	-7.809	-1.096	20.789			
	1.3	29.599	-8.129	-1.194	20.276			
	1.889	1.8	24.500	-7.443	-2.282	14.775	1.889	14.419
		1.9	24.353	-7.454	-2.474	14.425		
		2.0	25.408	-7.774	-2.654	14.980		

	$\rho$	$k$	$\epsilon_0$	$\epsilon_{2a}$	$\epsilon_{2b}$	$\epsilon$	$k_{cx}$	$\epsilon_{cx}$
MS	2.180	1.0	31.953	-8.225	-1.299	22.429	1.112	22.712
		1.1	33.212	-9.121	-1.382	22.709		
		1.2	33.769	-9.744	-1.487	22.538		
		1.9	24.492	-8.104	-3.745	12.643	1.976	12.270
		2.0	24.604	-8.171	-4.125	12.308		
		2.1	26.315	-8.745	-4.298	13.272		
	2.398	1.0	36.557	-10.513	-1.714	24.330	1.089	24.559
		1.1	37.939	-11.555	-1.828	24.556		
		1.2	38.394	-12.208	-1.974	24.212		
		2.0	24.249	-8.751	-6.202	9.296	2.052	9.064
		2.1	24.946	-9.044	-6.649	9.253		
		2.2	27.583	-10.011	-6.687	10.885		
	2.616	1.0	41.445	-13.563	-2.190	25.692	1.052	25.748
		1.1	42.922	-14.883	-2.338	25.701		
		1.2	43.520	-15.708	-2.511	25.301		
2.0		24.532	-9.560	-8.940	6.032	2.118	4.555	
2.1		23.979	-9.366	-10.017	4.596			
2.2		25.614	-10.071	-10.275	5.268			

Maxon and roton excitation spectrum calculated from relation (16). All energies are given in  $10^{-23}$  J, density in  $10^{28}$   $m^{-3}$  and the wave vector in  $10^{10}$   $m^{-1}$ . The notations of potentials are as follows: LJ (Lennard-Jones), BM (Bruch-McGee), FL (Farrar-Lee), B (Beck), A (Aziz et al.) and MS (Maitland-Smith).

TABLE 4.

	$\rho$	$k$	$\epsilon_0$	$\epsilon_{2a}$	$\epsilon_{2b}$	$\epsilon_{3a}$	$\epsilon_{4a}$	$\epsilon$
A	2.180	1.1	33.313	-9.073	-1.380	-0.296	-0.214	22.350
		2.0	24.532	-8.069	-4.123	-0.194	-0.731	11.465
	2.388	1.1	37.657	-11.293	-1.806	-0.482	-0.212	23.864
		2.0	24.230	-8.627	-6.086	-0.349	-0.580	8.588
	2.571	1.1	42.045	-13.680	-2.257	-0.751	-0.429	24.928
		2.1	24.102	-9.270	-9.219	-0.455	-0.577	4.591

Maxon and roton spectrum of Aziz potential calculated from relation (18); the notations and units are the same as in Table 3.

greater than  $2.82 \cdot 10^{28}$   $m^{-3}$ . (The lowest density of the solid  ${}^4\text{He}$  is  $\rho = 2.844 \cdot 10^{28}$   $m^{-3}$ ). The experimental threshold energy corresponds to the pressure of  $1.82 \cdot 10^6$  Pa<sup>16)</sup> (which is 18 times larger than the normal pressure), at temperature near 1 K, which gives the threshold density about  $2.52 \cdot 10^{28}$   $m^{-3}$ . But experimental results show that a maxon, under the above conditions, retains its identity

at energies above the instability threshold energy ( $2\Delta_0$ ). We see that our approach, with one- and two-phonon basis functions, describes this experimental situation only qualitatively. In addition we can say that decay of a maxon into two rotons does not appear, although energy and momentum could be conserved. This result is also interpreted as a repulsive interaction between two roton<sup>2-17)</sup> for the total momentum of about  $10^{10} \text{ m}^{-1}$ .

As far as we know the best theoretical values (analytic approach) of  $\Delta_0$  have been obtained by Lee and Lee<sup>5)</sup>. They have used BW perturbation formula up to the fourth order at SVP density. In our generalized formula we summed up an infinite number of diagrams<sup>8)</sup>, but only with one and two phonons out of the condensate. A comparison of our results with those from Ref. 5 and the experimental ones<sup>16)</sup> shows that the role of other diagrams, with three (and more) phonons out of the condensate, is very important at higher densities as well.

The effects of triplet correlations, which are included in three body structure factors in the Feenberg form, are very important. The contribution of the triplet correlations, with respect to Jastrow's, in the maxon part is 16.6, 16.2, 19.3, 19.7 (%) and in the part of the spectrum 15, 18, 21, 26 (%) for densities 2.185, 2.388, 2.571 and 2.844 ( $10^{28} \text{ m}^{-3}$ ) respectively. Triplet effects in the roton part of the spectrum increase significantly with increasing density.

We also notice from Table 2 that at higher densities the improved formula does not give better results than the pure BW formula.

Now we turn to the analysis of Tables 3 and 4. As we see from Table 3 for all potentials we have qualitatively the same behaviour: with density increase the energy of a maxon is increased and the energy of a roton is decreased. The three-phonon states, described by  $\varepsilon_{2b}$  term, become very important at higher densities; this term has stronger effects in the roton part of the spectrum and it significantly depends upon the used potential. For instance the energy of a roton at the density of  $2.517 \cdot 10^{28} \text{ m}^{-3}$  for LJ potential is almost four times greater than the same for BM potential. In addition, the threshold density for LJ potential is 2.49 and 2.14 for BM potential (in  $10^{28} \text{ m}^{-3}$ ). All these differences show that experimental data at higher densities could be used as a good estimation of the quality of the chosen potentials.

From Table 4 (where the Feenberg approximation was used for  $S_3$  in the term  $\varepsilon_{3a}$ ) we find that terms of the third and fourth order represent 2—4% of the sum of the second order terms. It is interesting to notice an unexpected behaviour of the fourth order term. In the roton part of the spectrum the relative influence of it decreases with the density increase.

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## ZAVISNOST JEDNOČESTIČNIH POBUĐENJA U TEKUĆEM $^4\text{He}$ O GUSTOĆI, TRIPLETNIM KORELACIJAMA I RAZLIČITIM POTENCIJALIMA

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Koristeći se Brillouin-Wignerovom perturbacionom formulom, analizirali smo utjecaj različitih gustoća i potencijala na maxonski i rotonski dio spektra jednočestičnih pobuđenja u tekućem heliju 4. Također je razmotren utjecaj tripletnih korelacija u navedenim uvjetima. Pokazano je da trofononska međustanja u drugom redu Brillouin-Wignerova računa smetnje igraju važnu ulogu i to naročito pri povećanim gustoćama; ovo je bilo predviđeno u našim ranijim istraživanjima. Nadalje je dokazana znatna zavisnost spektra o korištenim potencijalima koja osobito dolazi do izražaja pri povećanim gustoćama. Utjecaj tripletnih korelacija također je značajan, prema očekivanju, u rotonskom dijelu spektra znatno raste sa gustoćom.